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Theory of ultrasonic attenuation in heavy fermion compounds

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tract . The mechanism of the ultrasonic attenuation in heavy fermion compounds is not yet studied clearly both experimentally and etically A microscopic theoretical model is proposed here to study the attenuation in the compounds like UPt_3, $CeCu_2Si_2$, $CeRu_2Si_2$ in their normal :s We consider the Periodic Anderson Model and incorporate phonon coupling to the hybridisation between the conduction electrons and ctrons as well as to the f-electrons alone The phonon Green's function is calculated by Zubarev technique The temperature dependence of the sonic attenuation coefficient (α) is calculated from the imaginary part of the phonon self-energy and the velocity of sound in the dynamic and wavelength limit The dependence of the parameters like the electron-phonon coupling parameters (g, r), hybridisation (v), position of f-level (d), lomb correlation (u), frequency (ω), is investigated numerically through plots

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Introduction

n after the discovery of heavy fermion superconductivity, asonic data have revealed power law dependence for nuation coefficients for $T < T_c$ and a maximum around ~0.5 K for UPt_3 is observed [1-3]. The attenuation maximum urs exactly where the elastic constant and the velocity of ind exhibit minima [4]. It is also observed that the pronounced asonic attenuation peak of URu_2Si_2 coincides with the middle the elastic constant step indicating that the maximum of α urs at $T_c \approx 1.2$ K.

The first attenuation measurements in zero magnetic field owing Kondo effect were done by Müller *et al* [5]. A peak in attenuation was seen at 10–12K [6]. Similar low temperature omalies were observed in the elastic constants and the ocity of sound for compounds $CeCu_6$ (T^* = 4K), $CeCuSi_2$ (T^* 0K), URu_2Si_2 (T^* = 70K), $CeBe_{13}$ (T^* = 340K) [7].

Thalmeier [8] has considered Grüneisen parameter coupling sound waves to the bands to explain the elastic anomalies in temperature quasi-particle resime. Others have considered strain-dependence of the hybridisation to investigate the temperature anomaly in sound velocity of heavy fermion systems by using a mean field approach [9]. Rout and Das [10] have calculated velocity of sound of superconducting heavy fermion systems. In this paper, a microscopic theoretical model is proposed to investigate the ultrasonic attenuation in normal state heavy fermion systems. The attenuation Müller peak [5] can be described in terms of a narrow resonance peak with width of ~ 2 meV in the density of state lying above the Fermi surface resulting from the hybridisation of f-level and the conduction band.

2. Formalism

The system is described by the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{e-p} + \mathcal{H}_p , \tag{1}$$

$$\mathcal{H}_0 = \sum_{k,\sigma} \varepsilon_k c^{\dagger}_{k,\sigma} c_{k,\sigma} + \varepsilon_f \sum_{k,\sigma} f^{\dagger}_{k,\sigma} f_{k,\sigma}$$
$$+V \sum_{k,\sigma} \left(f^{\dagger}_{k,\sigma} c_{k,\sigma} + c^{\dagger}_{k,\sigma} f_{k,\sigma} \right)$$
$$+(U/2) \sum_{i,\sigma} n^f_{i,\sigma} n^f_{i,-\sigma} . \tag{2}$$

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$$\mathcal{H}_{e-p} = \sum_{\kappa,q,\sigma}\Big[f_1(q)\left(c^{\dagger}_{\kappa+q,\sigma} f_{\kappa,\sigma} + f^{\dagger}_{\kappa+q,\sigma} c_{\kappa,\sigma}\right)$$

$$+f_2(q)\left(f^{\dagger}_{\kappa+q,\sigma} f_{\kappa,\sigma}\right)\Big]\left(b_q + b^{\dagger}_{-q}\right), \tag{3}$$

$$\mathcal{H}_p = \sum_q \omega_q b^{\dagger}_q b_q . \tag{4}$$

$\mathcal{H}_0$, $\mathcal{H}_{e-p}$ and $\mathcal{H}_p$ are the Hamiltonians representing Periodic Anderson Model, electron-phonon interaction and free phonon term. Here $c^{\dagger}_{\kappa,\sigma}(c_{\kappa,\sigma})$ $f^{\dagger}_{\kappa,\sigma}(f_{\kappa,\sigma})$, $b^{\dagger}_q(bq)$ are the creation (annihilation) operators of d- and f- electrons and phonons respectively. ε_k, ε_f and V are the conduction electron energy, position of f-level and hybridisation respectively. U is the Coulomb interaction. $f_1(q)$ and $f_2(q)$ are the phonon coupling to hybridisation and f-electron respectively.

The double time Green's function of Zubarev type is defined as

$$D_{q,q}(t-t') = -i\Theta(t-t')\left\langle\left[A_q(t)\,;\,A_q(t')\right]\right\rangle . \tag{5}$$

Applying Dyson's approximation, the phonon Green function can be written as

$$D_{q,q}(\omega) = \left(\omega_q/\pi\right)\left[\omega^2 - \omega_q^2 - \Sigma_q(\omega)\right]^{-1}, \tag{6}$$

where phonon self energy is given by

$$\Sigma_q(\omega) = 4\pi\,\omega_q \chi_{q,q}(\omega),$$

$$\chi_{q,q}(\omega) = \Sigma_{\kappa,\sigma}\Big[f_1^2(q)\,\Gamma_3 + f_1(q)\,f_2(q)\left(\Gamma_4 + \Gamma_5\right)$$

$$+f_2^2(q)\,\Gamma_6\Big]. \tag{7}$$

$\Gamma_i(k,q,\omega)$'s (i = 3 to 6) represent the electron response functions. They are defined by dropping k, q, ω in terms of α's and β's as

$$\Gamma_3 = \ll\left(\alpha^a + \alpha^b\right);\left(\beta^a + \beta^b\right)\gg_\omega ,$$

$$\Gamma_4 = \ll\left(\alpha^a + \alpha^b\right);\beta^c\gg_\omega ,$$

$$\Gamma_5 = \ll\alpha^c\,;\left(\beta^a + \beta^b\right)\gg_\omega ,$$

$$\Gamma_6 = \ll\alpha^c\,;\beta^c\gg_\omega . \tag{8}$$

These operators are written in abreviated form as

$$\alpha^a = c^{\dagger}_{k-q,\sigma} f_{k,\sigma},\quad \alpha^b = f^{\dagger}_{k-q,\sigma} c_{k,\sigma},$$

$$\alpha^c = f^{\dagger}_{k-q,\sigma} f_{k,\sigma},\quad \alpha^d = c^{\dagger}_{k-q,\sigma} c_{k,\sigma} .$$

$$\left(\beta^a + \beta^b\right) = c^{\dagger}_{k'-q',\sigma'} f_{k',\sigma'} + f^{\dagger}_{k'-q',\sigma'} c_{k',\sigma'},$$

$$\beta^c = f^{\dagger}_{k'-q',\sigma'} f_{k',\sigma'} .$$

In the long wavelength limit, $q \to 0$. One has $\omega =$ and $\omega_0 = v_0 q$ where v_0 and v are the bare and renormali longitudinal sound velocities. The velocity of sound is gi by

$$v = v_0\left[1 + \frac{4\pi\chi(\omega,q)}{\omega_0}\right]^{1/2}$$

The ultrasonic attenuation coefficient $\alpha(\omega,T)$ for so waves of frequency ω and at a temperature T is obtained fr the imaginary part of self energy through

$$\alpha(\omega,T) = -\frac{4\pi}{}\,\mathrm{Im}\,\chi(\omega,q), \qquad ($$

where the -ve sign indicates absorption of energy. To st ultrasonic attenuation, the parameters are made dimension with respect to Debye frequency ω_D.

$$\tilde{\omega} = \frac{\omega}{\omega_D},\ c = \frac{\omega}{\omega_D},\ p = \frac{\omega_0}{\omega_D},\ e = \frac{\eta}{\omega_D},\ d = \frac{\varepsilon_f}{\omega_D};$$

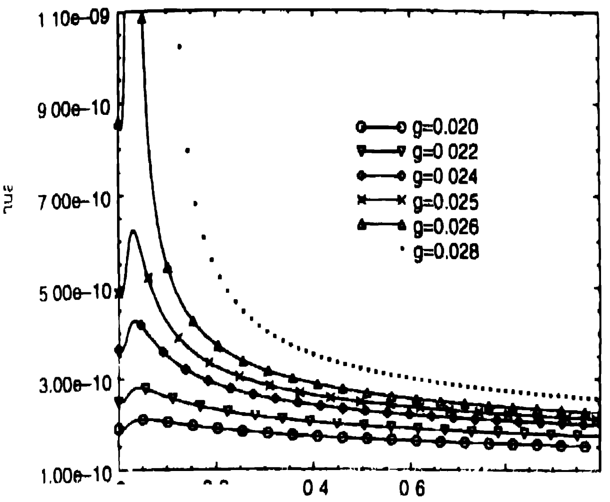
$$u = \frac{U}{\omega_D},\ d_1 = d + un,\ V = \frac{V}{\omega_D},\ g = \frac{N(0)\,f_1(0)^2}{\omega_D}$$

$$r = \frac{f_2(0)}{f_1(0)},\ t = \frac{kT}{\omega_D},\ \tilde{\omega}_i = \frac{\omega_i}{\omega_D},\ x = \frac{\varepsilon_k}{\omega_D},\ \tilde{W} = \frac{W}{\omega_D}$$

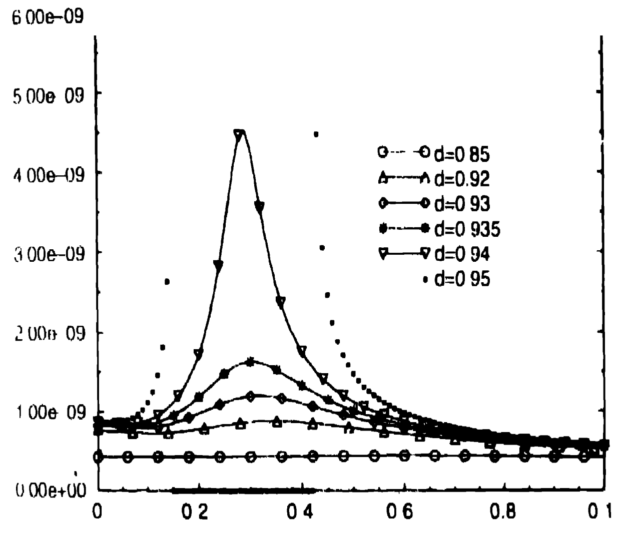
3. Results and discussion

The velocity of sound is evaluated numerically under half-fil band situation. The Fermi level is taken at the middle of band with $\varepsilon_F = 0$. The dimensionless parameters involve numerical calculations are the phonon coupling strength the ratio (r) between the phonon coupling to hybridisation the f-level, the position of the bare f-level (d), hybridisation Coulomb interaction (u). The temperature variation of ultrasonic attenuation of sound of the heavy fermion syste shows unusually high anomaly at low temperatures for cer physical parameters. The anomaly is discussed below.

Figure 1 shows the variation of ultrasonic attenuation temperature. As phonon coupling (g) to the hybridisat increases, the ultrasonic absorption increases and as a res peak height increases near temperature t = 0.05. With De frequency $\omega_D \approx$ 200K, this corresponds to fluctuat temperature $T^* \approx$ 10K. The phonon coupling increases hybridisation between f-electron and conduction band results in increase of mixed valence behaviour. When effec evel lies below the Fermi level, the attenuation decreases with crease of phonon coupling (r) to the f-electron alone.



igure 1 The variation of ultrasonic attenuation with temperature for fferent values of g = 0 020, 0 022, 0 024, 0 025, 0.026, 0 028 and fixed alues of r = 0, d = -0 94, v = 0 05, u = 1 0, e = 0 005, p =0.12.



igure 2. The variation of ultrasonic attenuation with temperature for fferent values of d = - 0 85, -0 92, 0.93, -0.935, -0 94, 0 95 and xed values of g = 0 026, r = 0, v = 0 05, u = 1 0, e = 0.005, p = 0 12

Figure 2 shows the variation of attenuation peak with temperature. As f-level moves from d = – 0.85 to – 0.95 from above, towards the Fermi level $\varepsilon_F = 0$, the attenuation increases and attenuation maximum shifts to lower temperature. The shifting of f-level in the conduction band changes the hybridisation between d- and f-electrons. This leads to change in the density of states near Fermi level and changes the fluctuation temperature (T^*). Hence, the ultrasonic attenuation and softening elastic constant of several heavy fermion compounds can be explained.

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